Peter Yatsyshin

Fellow of the Higher Education Academy (FHEA)

Honorary Fellow at Imperial College London

Research Associate at The Alan Turing Institute

Email: pyatsyshin@turing.ac.uk
p.yatsyshin@imperial.ac.uk

Phone: +44 (0)7476 209526

Address: The Alan Turing Institute
British Library, 96 Euston Road,
London NW1 2DB, UK

Curriculum Vitae

June 2022

Education

2014	Ph.D.	Department of Chemical Engineering, Imperial College London, UK *Ph.D. granted on March 1, 2014*
2007	M.Sc. (Hons)	Department of Physics and Mechanics, Peter the Great Saint-Petersburg Polytechnic University[1], Russia University Web Page: https://english.spbstu.ru *Distinction earned converts to UK first-class honours*
2005	B.Sc. (Hons)	Department of Physics and Mechanics, Peter the Great Saint-Petersburg Polytechnic University[1], Russia *Distinction earned converts to UK first-class honours*
2001	High School	Second Saint-Petersburg Gymnasium, Russia

Appointments

2020 –	**Postdoctoral Research Associate**, Data-centric Engineering group, The Alan Turing Institute, UK
2014 – 2019	**Postdoctoral Research Associate**, Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London, UK
2012–2014	**Research Assistant**, Complex Multiphase Systems Group, Department of Chemical Engineering, Imperial College London, UK
2009–2012	**Marie-Curie Early Stage Researcher**, Complex Multiphase Systems Group, Department of Chemical Engineering, Imperial College London, UK
2007–2009	**Researcher**, Faculty of Physics and Mechanics, Saint-Petersburg State Polytechnic University, Russia

Awards and recognition

2019 **Assistant Supervisor**. This officially recognises my involvement in training PhD students at the departments of Mathematics and Chemical Engineering at Imperial College London

2018 **Fellow of The Higher Education Academy** (FHEA). Recognition reference: PR147264. This is a *"recognition of attainment against the UK Professional Standards Framework for teaching and learning support in higher education."*

2017 **Sir William Wakeham Award** given by the Department of Chemical Engineering at Imperial College. This is the highest departmental honour, which annually recognises one or two *"early-career researchers... who have made a significant contribution to their research field."* The selection is made by an independent professorial panel. Click on links below for more info.
Award web page with a list of winners by year News article about the winners in 2017

2009 **Saint-Petersburg Government Award** for outstanding post-graduate students and early stage researchers from institutions located in the Saint-Petersburg Federal District.

[1] This is one of the top Russian universities and research centers in the fields of physics, applied maths and engineering. It was founded in 1899 as the most advanced engineering school in Russia at the time (Wikipedia page). Currently it ranks as 11th in Russia. Unfortunately, Russian universities do not regularly participate in international rankings. Nevertheless, some ranking info is provided on the university website: https://english.spbstu.ru/university/.

Research funding

2017 Imperial College European Partners Fund "*Density-functional modelling of nanofluidic systems*." This funding is for short academic visits to collaborators in Europe.
Co-investigator with Prof. Serafim Kalliadasis. Duration: 24 months. Amount: £4,400

2016 Imperial College "EPSRC Pathways to Impact Awards" (web link). This is an Imperial College impact acceleration funding scheme. I wrote the research proposal "*Interactive library for classical density-functional theory modeling of soft matter*," based on my numerical work on modelling equilibrium and dynamics of interfaces and soft matter. Due to the nature of my employment (postdoc), I was officially the co-investigator to my supervisor Prof. Serafim Kalliadasis. Duration: 12 months. Amount: £57,977

2016 COST (www.cost.eu) Short Term Scientific Mission "*Density functional modeling of formation, stability and dynamics of nanodroplets*". This was a research secondment. I have written the proposal for it and was the principal investigator. The host was Prof. Detlef Lohse, University of Twente, Enschede (Netherlands). Duration: 1 month. Amount: €1,000 [Due to some admin problems, funds have not been released as of yet.]

2014 Travel grant to attend Flow 14 – 1-st International Conference on Micro- and Nanofluidics Fundamentals and Applications, Enschede, Netherlands. Amount: €300

Teaching [My FHEA reference number: PR147264]

2017 - 2019 Lecturer for part of the two-semester course CE1-07 "Mathematics 1" (web link) for 1-st year Chemical Engineering undergraduates (~130 students), Imperial College
This course consists of 55 lectures across 5 modules: Analysis, Complex Numbers, Integration, Linear Algebra, ODEs. On any given year I taught 1–3 modules (15–35 lectures) and moderated assessments on all modules. I designed and delivered my own lectures; designed and marked final assessments; instructed GTAs; provided support across all modules to students via the online Blackboard Learn system, email and in-person meetings. I also moderated exam questions across all modules.

2015 - 2018 Lecturer for the part of the course CE4-09 "Dynamical Systems in Chemical Engineering" (web link) for 4-th year Chemical Engineering undergraduates, Imperial College London, UK
Delivered 3 one-hour lectures on deterministic chaos. Moderated final assessments.

2015 Lecturer, GTA and tutor at the course CE1-03-4 "Introduction to MATLAB" (web link) for 1-st year Chemical Engineering undergraduates (~ 130 students), Imperial College
Delivered 4 one-hour lectures; one-to-one tutoring, co-designed and co-marked exams.

2009 Tutor at the mathematics course for 2-nd and 3-rd year Economics undergraduates, Saint-Petersburg State Polytechnic University, Russia
Solving problems in linear algebra, differential geometry, ODEs

2008 Tutor at the physics course for 1-st year Electrical Engineering undergraduates, Saint-Petersburg State Polytechnic University, Russia
Solving problems in classical mechanics

PhD Students Supervision

2016–2020 Assistant supervisor for PhD project of Antonio Russo
"Multi-phase fluids: Molecular dynamics, generalized Langevin equation and fluctuating dynamic density functional theory",
Department of Chemical Engineering, Imperial College London, UK
Main supervisor: Prof Serafim Kalliadasis

2017–2019 Assistant supervisor for PhD project of Douglas Addy
"Cricital imperfect pitchfork bifurcations",
Department of Chemical Engineering, Imperial College London, UK
Main supervisor: Prof Serafim Kalliadasis

M.Sc. Students Supervision

Nov 2017– Jun 2018 Co-supervisor of M.Sc. project of Yujun Song
"Dynamical aspects of wetting by thin liquid films",
Department of Chemical Engineering, Imperial College London, UK
Co-supervisors: Dr Miguel Durán-Olivencia, Prof Serafim Kalliadasis

Nov 2015–Jun 2016 Co-supervisor of M.Sc. project of Titilayo Ruth Adeyinka
"Phase transitions and nucleation processes using density-functional theory",
Department of Chemical Engineering, Imperial College London, UK
Co-supervisors: Dr Miguel Durán-Olivencia, Prof Serafim Kalliadasis

Nov 2014–Jun 2015 Co-supervisor (unofficial) of M.Sc. project of Matteo Morciano
"Nonequilibrium molecular dynamics simulations of nanoconfined fluids at solid-liquid interfaces",
Department of Chemical Engineering, Imperial College London, UK
Co-supervisor: Prof Serafim Kalliadasis

Administrative and Conference-Related Activities

2015–2019 Post Doc Rep for Chemical Engineering. Duties include representing post-docs on departmental meetings, co-organising symposia and social events.
In 2015, -18 was nominate for the annual Postdoc Development Center Reps Award

2015– 2019 Co-organiser of the Annual Chemical Engineering Post-Doc Symposium, Imperial College London, UK

2018 Co-organiser of minisymposium "Fluctuating Complex Dynamical Systems", within the British Applied Mathematical Colloquium, University of St. Andrews, UK

2016 Co-organiser of minisymposium "Statistical Mechanical and Phase Field Modelling of Inhomogeneous Fluids", within the British Applied Mathematical Colloquium, University of Oxford, UK

Publications

Ph.D. thesis

Analysis of the phase behaviour of a nano-confined Lennard-Jones fluid using pseudo-spectral approach to classical density-functional models

P. Yatsyshin (2014). Ph.D. thesis. Imperial College London.
URL: http://hdl.handle.net/10044/1/24122

a. Refereed Research Articles

1. **Physics-constrained Bayesian inference of state functions in classical density-functional theory**

   P. Yatsyshin, S. Kalliadasis and Andrew B. Duncan (2022), *Journal of Chemical Physics* **156** 074105
   DOI: 10.1063/5.0071629

Link to NeurIPS workshop from 2020 with the short version of the article:
NeurIPS workshop version

2. **Surface nanodrops and nanobubbles: a classical density functional theory study**

   P. Yatsyshin and S. Kalliadasis (2021), *Journal of Fluid Mechanics* **913** 1

   DOI: 10.1017/jfm.2020.1167

3. **A finite-volume method for fluctuating dynamical density functional theory**

   A. Russo, S. P. Perez, M. A. Durán-Olivencia, P. Yatsyshin, J. A. Carrillo, S. Kalliadasisa (2021), *Journal of Computational Physics* **428** 1

   DOI: 10.1016/j.jcp.2020.109796

4. **Mixing-demixing transition in polymer-grafted spherical nanoparticles**

   P. Yatsyshin, N. G. Fytas and E. Theodorakis (2020), *Soft Matter* **16** 703

   DOI: 10.1039/c9sm01639b

5. **Memory effects in fluctuating dynamic density-functional theory: theory and simulations**

   A. Russo, M. A. Durán-Olivencia, P. Yatsyshin and S. Kalliadasis (2020), *Journal of Physics A: Mathematical and Theoretical* **53** 445007

   DOI: 10.1088/1751-8121/ab9e8d

6. **Dynamics of the Desai-Zwanzig model in multiwell and random energy landscapes**

   S. N. Gomes, S. Kalliadasis, G. A. Pavliotis and P. Yatsyshin (2019), *Phys. Rev. E* **99** 032109

   DOI: 10.1103/PhysRevE.99.032109

7. **General framework for nonclassical nucleation**

   M. A. Durán-Olivencia, P. Yatshyshin, S. Kalliadasis and J. F. Lutsko (2018), *New J. Phys.* **20** 083019

   DOI: 10.1088/1367-2630/aad170

8. **Microscopic aspects of wetting using classical density-functional theory**

   P. Yatshyshin, M. A. Durán-Olivencia and S. Kalliadasis (2018), *J. Phys.: Condens. Matter* **30** 274003

   DOI: 10.1088/1361-648X/aac6fa

9. **Wetting of a plane with a narrow solvophobic stripe**

   P. Yatsyshin, A. O. Parry, C. Rascón and S. Kalliadasis (2018), *Mol. Phys.* **116** 1990

   DOI: 10.1080/00268976.2018.1473648

10. **General framework for fluctuating dynamic density functional theory**

    M. A. Durán-Olivencia, P. Yatsyshin, B. D. Goddard and S. Kalliadasis (2017), *New J. Phys.* **19** 123022

    DOI: 10.1088/1367-2630/aa9041

11. **Nonequilibrium molecular dynamics simulations of nanoconfined fluids at solid-liquid interfaces**

    M. Morciano, M. Fasano, A. Nold, C. C. Braga, P. Yatsyshin, D. N. Sibley, B. D. Goddard, E. Chiavazzo, P. Asinari, and S. Kalliadasis (2017), *J. Chem. Phys.* **146** 244507

    DOI: 1.4986904

12. **Classical density functional study of wetting transitions on nanopatterned surfaces**

    P. Yatsyshin, A. O. Parry, C. Rascón and S. Kalliadasis (2017), *J. Phys.: Condens. Matter* **29** 094001

    DOI: 1361-648X/aa4fd7

13. **Pseudospectral methods for density functional theory in bounded and unbounded domains**
A. Nold, B. D. Goddard, P. Yatsyshin, N. Savva and S. Kalliadasis (2016), *J. Comp. Phys* **334** 639
DOI: 10.1016/j.jcp.2016.12.023
14. **Mean-field phenomenology of wetting in nanogrooves**
P. Yatsyshin and S. Kalliadasis (2016), *Mol. Phys.* **114** 2688
DOI: 10.1080/00268976.2016.1224393
15. **Complete Prewetting**
P. Yatsyshin, A. O. Parry and S. Kalliadasis (2016), *J. Phys.: Condens. Matter* **28** 275001
DOI: 10.1088/0953-8984/28/27/275001
[Article was highlighted by reviewers as being "particularly significant to the community" and is featured at the journal's news blog **JPhys+**. This is a blog for articles that have wider appeal and interest as well as scientific importance and covers research news from across the *Journal of Physics* series.
URL: https://jphysplus.iop.org/2016/06/23/derjaguin-in-flatland-prewetting-spreads-out/]
16. **Density functional study of condensation in capped capillaries**
P. Yatsyshin, N. Savva and S. Kalliadasis (2015), *J. Phys.: Condens. Matter* **27** 275104
DOI: 10.1088/0953-8984/27/27/275104
17. **Wetting of prototypical one- and two-dimensional systems: thermodynamics and density functional theory**
P. Yatsyshin, N. Savva and S. Kalliadasis (2015), *J. Chem. Phys.* **142** 034708
DOI: 10.1063/1.4905605
18. **Unification of dynamic density functional theory for colloidal fluids to include inertia and hydrodynamic interactions: derivation and numerical experiments**
B. Goddard, A. Nold, N. Savva, P. Yatsyshin, and S. Kalliadasis (2013), *J. Phys.: Condens. Matter* **25** 035101
DOI: 10.1088/0953-8984/25/3/035101
[Article featured as a news item on the Imperial College web site
URL: http://tinyurl.com/z9mm4rt, it was selected as a journal news item – labtalk,
URL: http://iopscience.iop.org/0953-8984/labtalk-article/51831 and was included in IOPselect
URL: http://iopscience.iop.org/0953-8984/25/3/035101/ which contains a compendium of papers appearing in all IOP journals chosen by the editors for their "novelty, significance and potential impact on future research".]
19. **Geometry-induced phase transition in fluids: Capillary prewetting**
P. Yatsyshin, N. Savva, and S. Kalliadasis (2013), *Phys. Rev. E (Rapid Comm)*, **87**, 020402(R).
DOI: 10.1103/PhysRevE.87.020402
20. **Spectral methods for the equations of classical density-functional theory: relaxation dynamics of microscopic films**
P. Yatsyshin, N. Savva, and S. Kalliadasis (2012), *J. Chem. Phys.*, **136**, 124113
DOI: 10.1063/1.3697471
21. **Structure of electron–positron clusters: Hartree–Fock approximation**
P. Yatsyshin, R. G. Polozkov, V. K. Ivanov, and A. V. Solovyov (2009), *Phys. Scr.*, **80**, 048126
DOI: 10.1088/0031-8949/80/04/048126

22. **Resonances in the cross section of photodetachment of $2p$ electrons from negative ions Na^-**

    V. K. Ivanov and P. I. Yatsyshin (2009), *Technical Physics*, **54**, 7

    DOI: 10.1134/S1063784209010022

b. Book Chapters

23. **Classical Density Functional Theory and Nanofluidics: Adsorption and the Interface Binding Potential**

    P. Yatsyshin, M.-A. Durán-Olivencia and S. Kalliadasis

    In: Klaus Sattler (ed) *21st Century Nanoscience. A Handbook* Chapter **14** CRC Press (2020)

    DOI: 10.1201/9780429347313-14

24. **Classical density-functional theory studies of fluid adsorption on nanopatterned planar surfaces**

    P. Yatsyshin and S. Kalliadasis (2018)

    In: L.L. Bonilla, E. Kaxiras and R. Melnik (eds) *Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications.* BIRS-16w5069 2016. Springer Proceedings in Mathematics & Statistics, vol 232. Springer, Cham

c. Conference Papers

25. **Data-driven density functional theory: a case for physics-informed learning**

    P. Yatsyshin, S. Kalliadasis and A. B. Duncan (2021)

    Machine Learning and the Physical Sciences Workshop at the 35th Conference on Neural Information Processing Systems (NeurIPS)

    Workshop website

    Conference Article

    Video Introduction

26. **Equilibrium fluid structures in prototypical nanosystems**

    P. Yatsyshin, N. Savva and S. Kalliadasis (2016),

    8th GRACM International Congress on Computational Mechanics, University of Thessaly, Volos (Greece), July 2015

    URL: http://8gracm.mie.uth.gr/Papers/Session%20D1-B2/P.%20Yatsyshin.pdf

d. Conference Abstracts

Invited talks and seminars

1. *Data-Driven Classical Density Functional Theory: A Case for Physics Informed Learning*, New directions in classical density functional theory workshop, International Center for Mathematical Sciences, UK, April 2021

   URL: https://www.icms.org.uk/events/workshops/cdft

   Video of presentation

2. *Machine-learning the DFT of a classical statistical-mechanical system: A case for physics-informed learning*, Density Functional Days in Tübingen, Tübingen University, Germany, September 2020

3. *Wetting on striped walls: interplay between pre-wetting and interface unbending*, Density Functional Days in Tübingen, Tübingen University, Germany, September 2019

4. *Statistical Mechanics of Wetting*, Open Statistical Physics, School of Mathematics and Statistics, Open University, UK, March 2018

5. *Computational statistical mechanical framework for soft condensed matter. Mean-field description of wetting at the nanoscale*, Chemical Engineering Postdoc Symposium, Department of Chemical Engineering, Imperial College London, UK, April 2017.
6. *A computational statistical-mechanical framework: Classical density functional theory with applications to phase transition in nano-confined fluids*, Department of Mathematics & Statistics, The Open University, UK, November 2016.
7. *Statistical Mechanics of classical fluids: Density functional theory and equilibrium and dynamics of wetting*, Physics of Fluids group, University of Twente, Enschede, The Netherlands, in October 2016.
8. *Wetting at the nanoscale. Equilibrium and dynamics*
Video available at URL: (the link below is clickable in the .pdf file)
http://www.birs.ca/events/2016/5-day-workshops/16w5069/videos/watch/201608301028-Yatsyshin.html,
2016 BIRS Workshop on Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications, in Banff, Alberta, Canada, August 2016.
9. *Implementing computations with equilibrium and dynamic classical density functional theory*, Department of Mathematical Sciences, Loughborough University, Leicestershire, UK, in May 2016.
10. *Classical density functional theory for Lennard-Jones fluids. Applications to wetting on planar and sculpted substrates*, Molecular Systems Engineering group, Imperial College London, UK, in April 2016.
11. *Density functional theory for surface tensions and more*, presented within the four-part seminar "Exploration of fluids", Imperial College London, October 2014, chaired by Prof. S. H. Davis, Northwestern University, Royal Academy of Engineering Visiting Professor to the Department of Chemical Engineering, Imperial College London.
12. *Geometry-induced phase transitions*, Chemical Engineering Ph.D. symposium, Imperial College London, UK, June 2013.

Contributed talks

13. M. A. Durán-Olivencia, A. Russo, Yatsyshin, P. and S. Kalliadasis *Memory effects in fluctuating dynamic density-functional theory: theory and simulations*, 74th Annual Meeting of the APS Division of Fluid Dynamics, Phoenix (ARI, USA), November 2021
14. Yatsyshin, P., S. Kalliadasis, and A. B. Duncan *Data-Driven Classical Density Functional Theory: A Case for Physics Informed Learning*, APS March Meeting, Virtual meeting due to Covid-19 (USA), March 2021
15. Yatsyshin, P., A. O. Parry, C. Rascón, M. A. Durán-Olivencia, and S. Kalliadasis *Phase transitions at the interfaces and in the bulk. Equilibrium and dynamics studies using classical density functional theory*, Liblice 2018 (Czech Republic), June 2018
16. Yatsyshin, P., M. A. Durán-Olivencia, A. O. Parry, C. Rascón and S. Kalliadasis *Understanding interfacial wetting transitions with classical density functional theory*, APS March Meeting, Los Angeles (CA, USA), March 2018
17. Yatsyshin, P., A. O. Parry, C. Rascón and S. Kalliadasis *Wetting of chemically nanopatterned walls*, Workshop of the Fundamental Theoretical Approaches to the Equation of State, Manchester (UK), January 2018
18. Yatsyshin, P., A. O. Parry, C. Rascón, M. A. Durán-Olivencia, and S. Kalliadasis *Wetting of heterogeneous substrates. A classical density-functional-theory approach*, 70th Annual Meeting of the APS Division of Fluid Dynamics, Denver (CO, USA), November 2017
19. Yatsyshin, P., M. A. Durán-Olivencia, A. O. Parry, C. Rascón and S. Kalliadasis *Mean-field treatment of wetting at the nanoscale*, to be given at the summer school Complex Motion in Fluids 2017, Cambridge (UK), September 2017

20. Yatsyshin, P., A. O. Parry, C. Rascón and S. Kalliadasis *Classical density functional study of wetting transitions on nanopatterned surfaces*, Thermodynamics 2017, Edinburgh (UK), August 2017
21. Yatsyshin, P., M. A. Durán-Olivencia, A. O. Parry, C. Rascón and S. Kalliadasis *Wetting in flatland: Complex interfacial transitions at inhomogeneous solid-gas interfaces*, APS March Meeting, New Orleans (LA, USA), March 2017
22. Yatsyshin, P., D. N. Sibley, M. A. Durán-Olivencia and S. Kalliadasis, *Dynamics of two-phase interfaces and surface tensions: A density-functional theory perspective*, 69th Annual Meeting of the APS Division of Fluid Dynamics, Portland (OR, USA), November 2016
23. Yatsyshin, P., N. Savva, A. Nold, B. D. Goddard and S. Kalliadasis, *Mapped-Chebyshev spectral collocation approach to the integral and integral-differential equations of the classical equilibrium and dynamic density functional theory*, British Applied Mathematical Colloquium, University of Oxford, Oxford (UK), April 2016
24. Yatsyshin, P., A. O. Parry and S. Kalliadasis, *A computational DFT study of structural transitions in textured solid-fluid interfaces*, 68th Annual Meeting of the APS Division of Fluid Dynamics, Boston (MA, USA), November 2015
25. Yatsyshin, P., D. N. Sibley, N. Savva and S. Kalliadasis, *Molecular-level description of nano-drops: contact angles, dynamics of wetting and coalescence*, Droplets 2015, University of Twente, Enschede (Netherlands), October 2015
26. Yatsyshin, P., N. Savva and S. Kalliadasis, *Thermodynamics and statistical mechanics of wetting transitions: fluid phase behavior in prototypical nanostructured substrates*, Thermodynamics 2015, Technical University of Denmark, Copenhagen (Denmark), September 2015
27. Yatsyshin, P., N. Savva and S. Kalliadasis, *Equilibrium fluid structures in prototypical nanosystems*, 8th GRACM International Congress on Computational Mechanics, University of Thessaly, Volos (Greece), July 2015
28. Yatsyshin, P., D. N. Sibley, N. Savva and S. Kalliadasis, *Droplets and the three-phase contact line at the nano-scale. Statics and dynamics*, 67th Annual Meeting of the APS Division of Fluid Dynamics, San Francisco (CA, USA), November 2014
29. Yatsyshin, P., N. Savva and S. Kalliadasis, *Capillary Condensation Revisited: Wetting on a Capped Capillary*, Thermodynamics 2013, University of Manchester, Manchester (UK), September 2013
30. Yatsyshin, P., N. Savva and S. Kalliadasis, *Micro confined inhomogeneous fluids. Wetting on a capped capillary*, British Applied Mathematical Colloquium, University of Leeds, Leeds (UK), April 2013
31. Yatsyshin, P., N. Savva and S. Kalliadasis, *Relaxational Dynamics of Microscopic films. Spectral Methods for the Equations of Classical Density Functional Theory*, Summer School on Wave Patterns and Interactions in Advection-Dominated Flows, University of Thessaly, Volos (Greece), July 2012
32. Yatsyshin, P., N. Savva and S. Kalliadasis, *Integral and Integral-Differential equations of classical density functional theory. A novel numerical approach*, British Applied Mathematical Colloquium, University College London, London (UK), March 2012
33. Yatsyshin, P., N. Savva and S. Kalliadasis, *Dynamics of a thin film layer on planar substrate obtained from a dynamic density functional theory approach*, International Conference on Multiscale Complex Fluid Flows and Interfacial Phenomena, Free University of Brussels, Brussels (Belgium), November 2010